From localization to delocalization in the quantum Coulomb glass

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Abstract

We numerically investigate how electron-electron interactions influence the transport properties of disordered electrons in two dimensions. Our study is based on the quantum Coulomb glass model appropriately generalized to include the spin degrees of freedom. In order to obtain the low-energy properties of this model we employ the Hartree-Fock based diagonalization, an efficient numerical method similar to the configuration interaction approach in quantum chemistry. We calculate the d.c. conductance by means of the Kubo-Greenwood formula and pay particular attention to the spin degrees of freedom. In agreement with earlier results we find that electron-electron interactions can cause delocalization. For spinful electrons this delocalization is significantly larger than for spinless electrons.

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I. INTRODUCTION

The discovery of a metal-insulator transition (MIT) in the two-dimensional electron gas in Si-MOSFETs [1] has induced renewed attention to the transport properties of disordered electrons. This MIT is in conflict with the theory of localization for *non-interacting* electrons which predicts that all states are localized in 2D. The electron density in the Si-MOSFETs is very low which makes the electron-electron interaction particularly important. Thus it is generally assumed that some type of interaction effect is responsible for this MIT. One of the most remarkable findings about the MIT in Si-MOSFETs is that an in-plane magnetic field (which does not couple to the orbital motion of the electrons) strongly suppresses the conducting phase [2]. This suggests that the spin degrees of freedom play an important role for the transition. A complete understanding has, however, not yet been obtained. There have been attempts to explain the experiments based on the perturbative renormalization group [3], non-perturbative effects [4], or the transition being a superconductor-insulator transition rather than a MIT [5].

In order to attack the problem of disordered interacting electrons numerically we have developed [6,7] an efficient method, the Hartree-Fock based diagonalization (HFD) which is related to the quantum-chemical configuration interaction approach. We have used this method to study the influence of interactions on the conductance in one [8], two [6], and three [9] dimensions. We found a delocalizing tendency of the interactions for strong disorder but a localizing one for weak disorder. Similar results have been obtained by means of the density-matrix renormalization group [10] in one dimension and exact diagonalization in two dimensions [11]. Since in most of the numerical work in the literature spinless electrons were considered, there are not many results about the importance of the spin degrees of freedom.

In this work we address this question by generalizing the HFD method to spinful electrons. We then use it study the influence of the spin degrees of freedom on the Kubo-Greenwood conductance.

II. MODEL AND METHOD

The generic model for *spinless* interacting disordered electrons is the quantum Coulomb glass [12]. In this paper we use a straight-forward generalization of the quantum Coulomb glass to spinful electrons. It is defined on a regular hypercubic lattice with $g = L^d$ (d is the spatial dimensionality) sites occupied by $N = N_\uparrow + N_\downarrow = 2Kg$ electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of $2Ke$. The Hamiltonian is given by

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + \sum_{i,\sigma} \varphi_i n_{i\sigma} + \frac{1}{2} \sum_{i \neq j, \sigma, \sigma'} (n_{i\sigma} - K)(n_{j\sigma'} - K) U_{ij} + U_H \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where $c^\dagger_{i\sigma}$ and $c_{i\sigma}$ are the creation and annihilation operators at site i and spin σ, and $\langle ij \rangle$ denotes all pairs of nearest-neighbor sites. t is the strength of the hopping term, i.e., the kinetic energy, and $n_{i\sigma}$ is the occupation number of spin state σ at site i. We parametrize the interaction $U_{ij} = e^2/r_{ij}$ by its value U between nearest-neighbor sites. The Coulomb repulsion between two electrons at the same site is described by the Hubbard interaction U_H

The random potential values φ_i are chosen independently from a box distribution of width $2W_0$ and zero mean. The boundary conditions are periodic and the Coulomb interaction is treated in the minimum image convention (which implies a cut-off at a distance of $L/2$).

A numerically exact solution of a quantum many-particle system requires the diagonalization of a matrix whose dimension increases exponentially with system size. This severely limits the possible sample sizes. In order to overcome this problem we have developed the HFD method. The basic idea is to work in a truncated Hilbert space consisting of the corresponding Hartree-Fock (Slater) ground state and the low-lying excited Slater states. For each disorder configuration three steps have to be performed: (i) find the Hartree-Fock solution of the problem, (ii) determine the B Slater states with the lowest energies, and (iii) calculate and diagonalize the Hamilton matrix in the subspace spanned by these states. The number B of new basis states determines the quality of the approximation, reasonable values have to be found empirically.

III. RESULTS

The conductance of a quantum many-particle system can be obtained from linear-response theory. It is essentially determined by the current-current correlation function of the ground state. The real (dissipative) part of the conductance (in units of e^2/h) is given by the Kubo-Greenwood formula [13],

$$\text{Re } G^{xx}(\omega) = \frac{2\pi^2}{\omega} \sum_{\nu} |\langle 0|j^x|\nu\rangle|^2 \delta(\omega + E_0 - E_\nu) \tag{2}$$

where ω denotes the frequency. j^x is the x component of the current operator and ν denotes the eigenstates of the Hamiltonian. Eq. (2) describes an isolated system while in a real d.c. transport experiment the sample is connected to contacts and leads. This results in a finite life time τ of the eigenstates leading to an inhomogeneous broadening $\gamma = \tau^{-1}$ of the δ functions in (2) [14]. To suppress the discreteness of the spectrum of a finite system, γ should be at least of the order of the single-particle level spacing. For our systems this requires a comparatively large $\gamma \geq 0.05$. We tested different γ and found that the conductance *values* depend on γ but the qualitative results do not.

The main results of this paper are summarized in Fig. 1 which shows the disorder and interaction dependence of the typical conductance for both spinless and spinful electrons on a two-dimensional lattice of 4×4 sites. The qualitative behavior in both cases is similar: In the strongly localized regime (small t) a moderate interaction delocalizes the electrons while a sufficiently strong interaction always strongly suppress the conductance. This is the precursor of a Wigner crystal or Wigner glass. With decreasing disorder (increasing t) the interaction-induced enhancement of the conductance also decreases and eventually vanishes. The behavior of the conductance can be attributed to the competition of two effects: First, the interactions destroy the phase of the electrons and thus the interference necessary for localization. This is particularly effective if the localization length is small to begin with. Second, the interactions introduce an additional source of randomness which tends to increase the localization.

A comparison of the cases of spinless and spinful electrons shows that the interaction induced delocalization is significantly larger for spinful electrons. Moreover, the enhancement

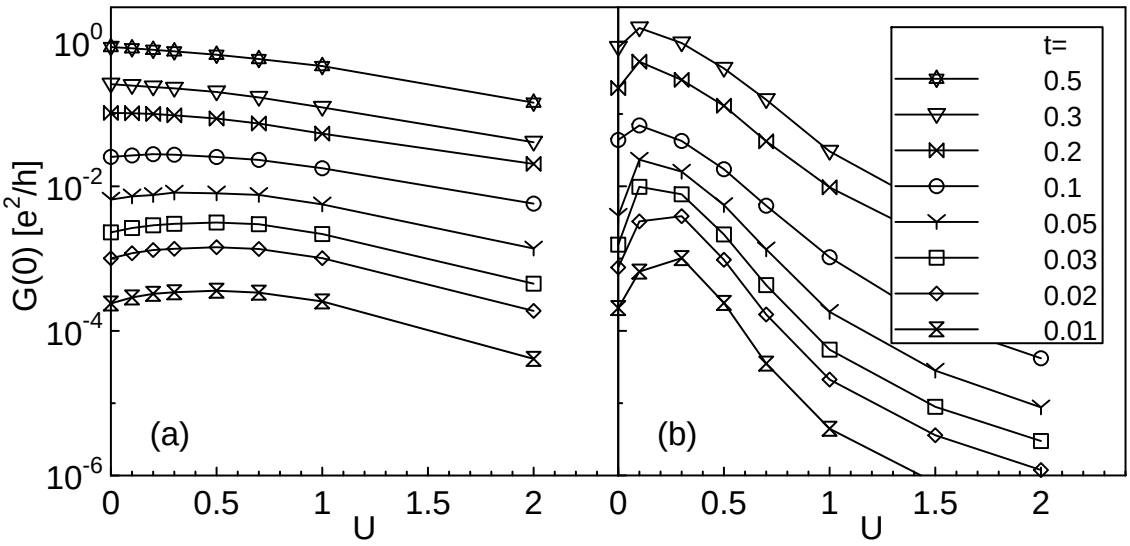

FIG. 1. d.c. conductance $G(0)$ for a system of 4×4 lattice sites occupied by (a) 8 spinless electrons or (b) 8 spin-up and 8 spin-down electrons for different U and t. The disorder strength is fixed to $W_0 = 1$, the Hubbard energy is $U_H = 0.5$, the broadening is $\gamma = 0.0625$, and the HFD basis size is $B = 500$. The data points represent logarithmical averages over 400 samples.

seems to vanish at a larger kinetic energy (which we did not reach in the simulations). A systematic investigation of the dependence of the conductance on U and U_H will be published elsewhere.

In summary, we have studied the influence of electron-electron interactions on Anderson localization for spinless and spinful electrons in two dimensions. For strong disorder moderate interactions significantly enhance the transport. This enhancement is much stronger for spinful than for spinless electrons. Identifying a real phase transition and thus establishing a connection between these findings and the experiments on Si-MOSFETs requires a finite-size scaling analysis of the conductance. This remains a task for the future.

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